Supporting Information

Complexes with Redox-Active Ligands: Synthesis, Structure, Electrochemical and Photophysical Behavior of Ru(II) Complex with TTF-Annulated Phenanthroline

Lawrence K. Keniley Jr.,[†] Nathalie Dupont,[‡] Lipika Ray,[†] Jie Ding,[‡] Kirill Kovnir,[†,§] Jordan M. Hoyt,[†,#] Andreas Hauser,[*,‡] Michael Shatruk[*,†]

[†]*Department of Chemistry and Biochemistry, Florida State University, 95 Chieftan Way, Tallahassee, FL 32306, USA*

[‡]*Department of Physical Chemistry, University of Geneva, 30 quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland*

[§] *Present address: Department of Chemistry, University of California at Davis, Davis, CA 95616, USA*

[#] *Present address: Department of Chemistry, Princeton University, Princeton, NJ 08544, USA*

E-mail: shatruk@chem.fsu.edu, andreas.hauser@unige.ch

Figure S1. ^{1}H and 2D COSY NMR spectra of **1**, **2**, and **3** S2

Figure S2. The proximity of the α-protons to the π-system of bpy S5

Figure S3. Crystal packing of **L1** S5

Figure S4. Emission spectra of complexes **1**-**3** S6

Figure S5. Kinetic profile of the difference absorbance spectrum of **1** S7

Figure S6. Absorption and emission spectra of a control CH_3CN solution of **1** S7

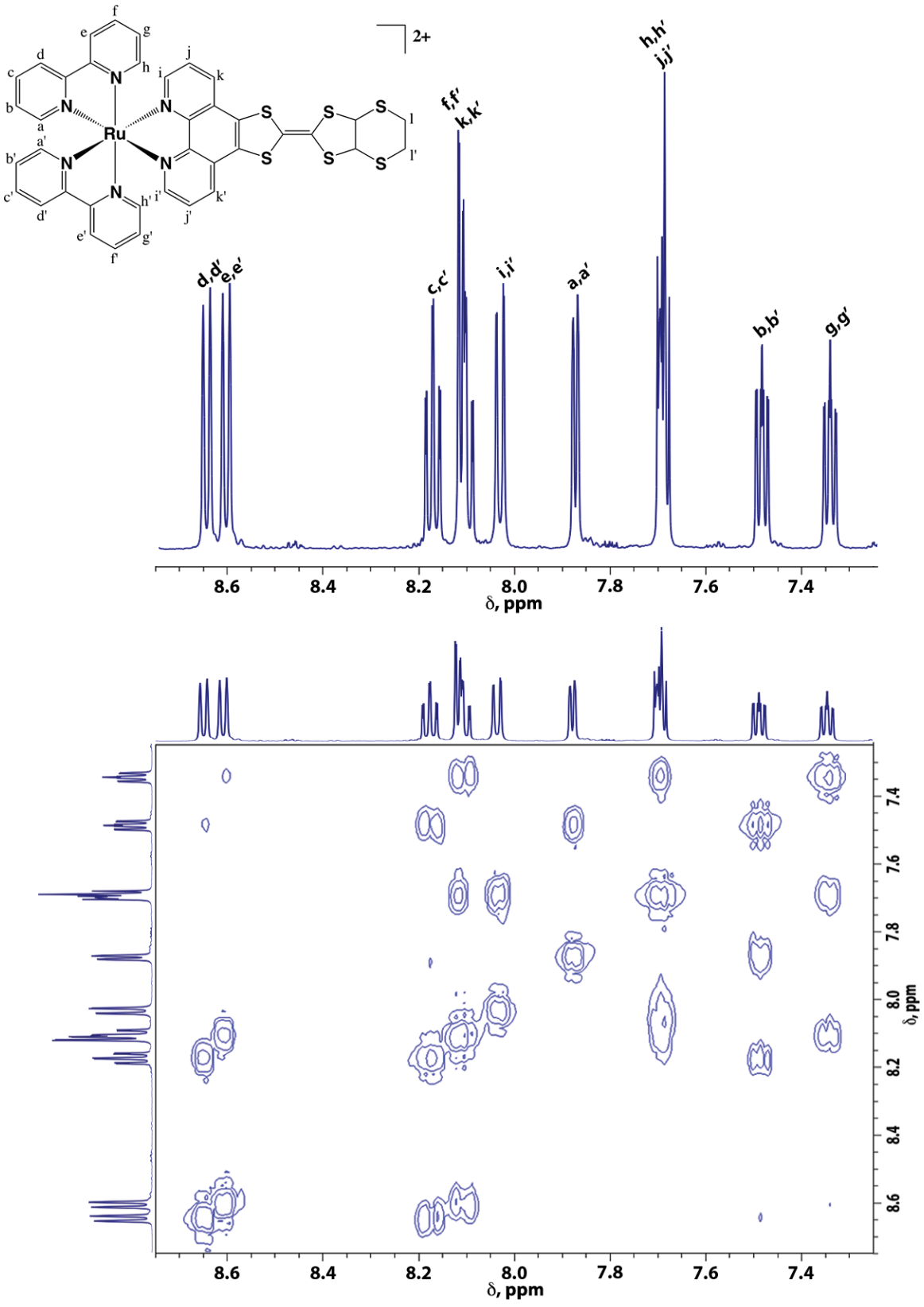

Figure S1. ^{1}H and 2D COSY NMR spectra of **1**, **2**, and **3** in $CDCl_3$ at room temperature.

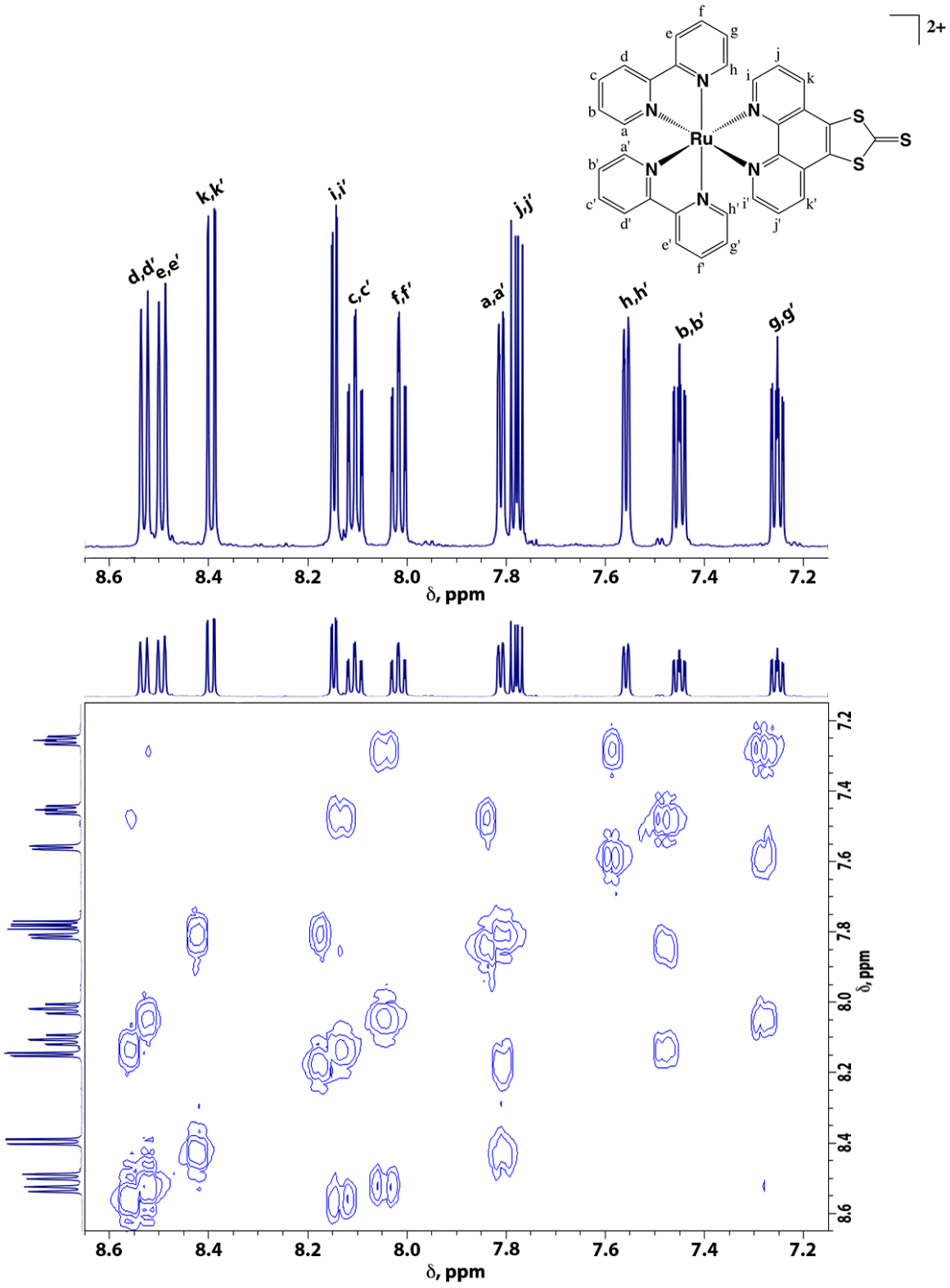

Figure S1 (continued). ^{1}H and 2D COSY NMR spectra of **1**, **2**, and **3** in $CDCl_3$ at room temperature.

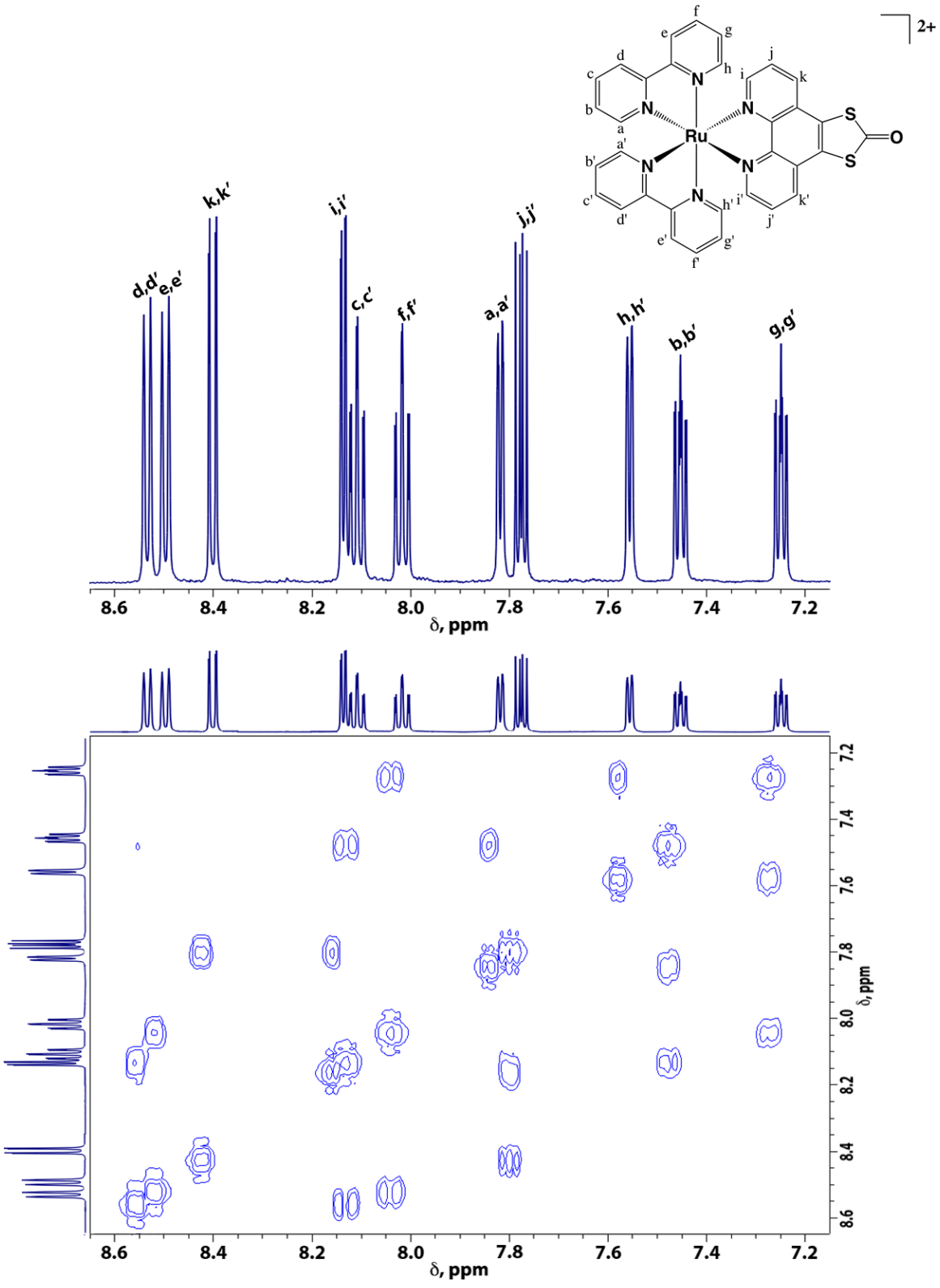

Figure S1 (continued). ^{1}H and 2D COSY NMR spectra of **1**, **2**, and **3** in $CDCl_3$ at room temperature.

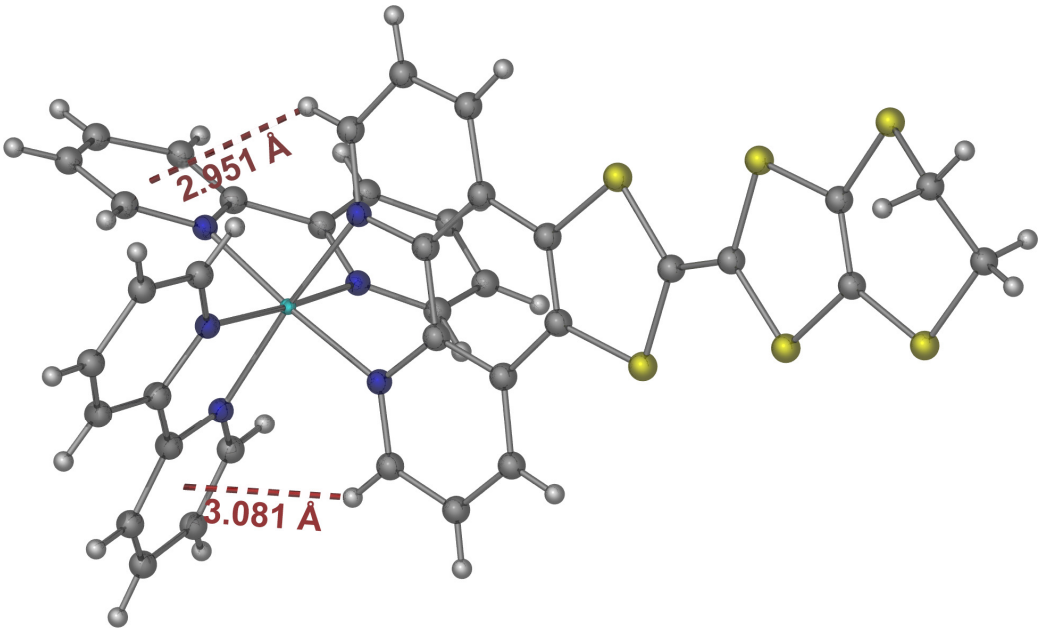

Figure S2. Molecular structure of $[Ru(bpy)_2(\mathbf{L1})]^{2+}$ showing the proximity of the α-protons of coordinated **L1** to the π-system of bpy ligands.

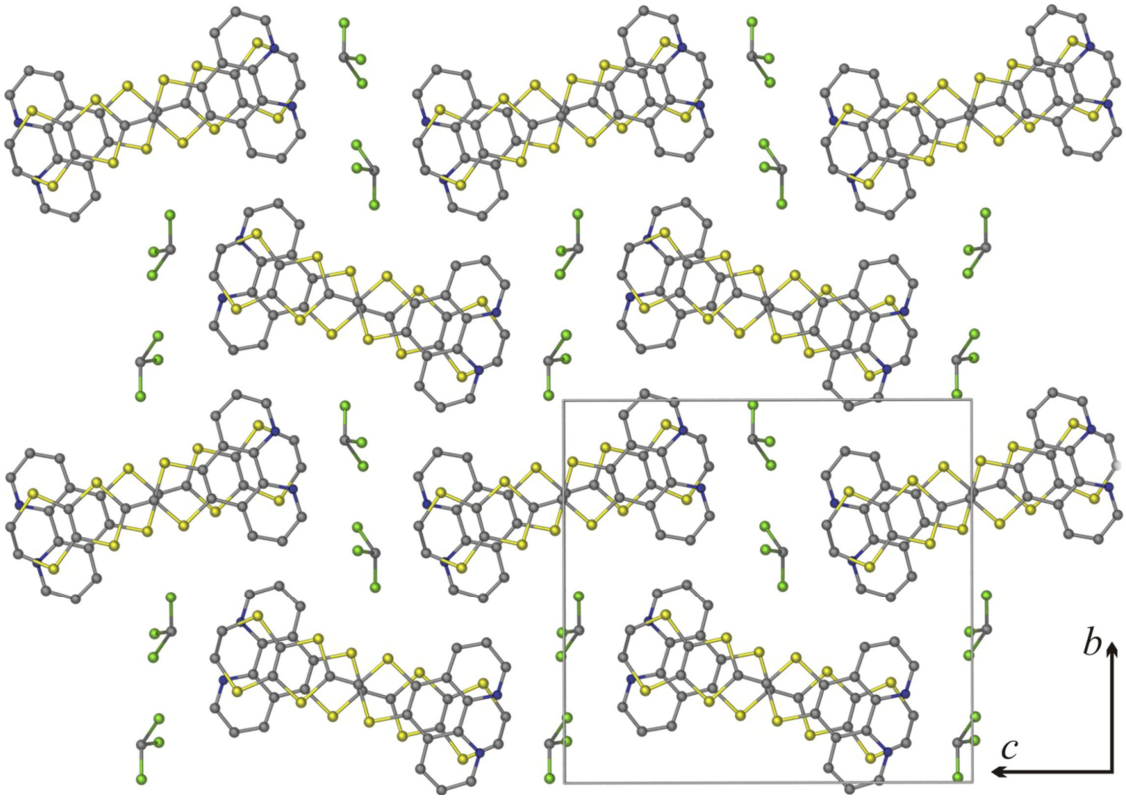

Figure S3. Crystal packing of **L1** illustrating the columns of molecules stacked in a head-to-tail fashion. The columns run parallel to the *a* axis. H atoms are omitted for clarity.

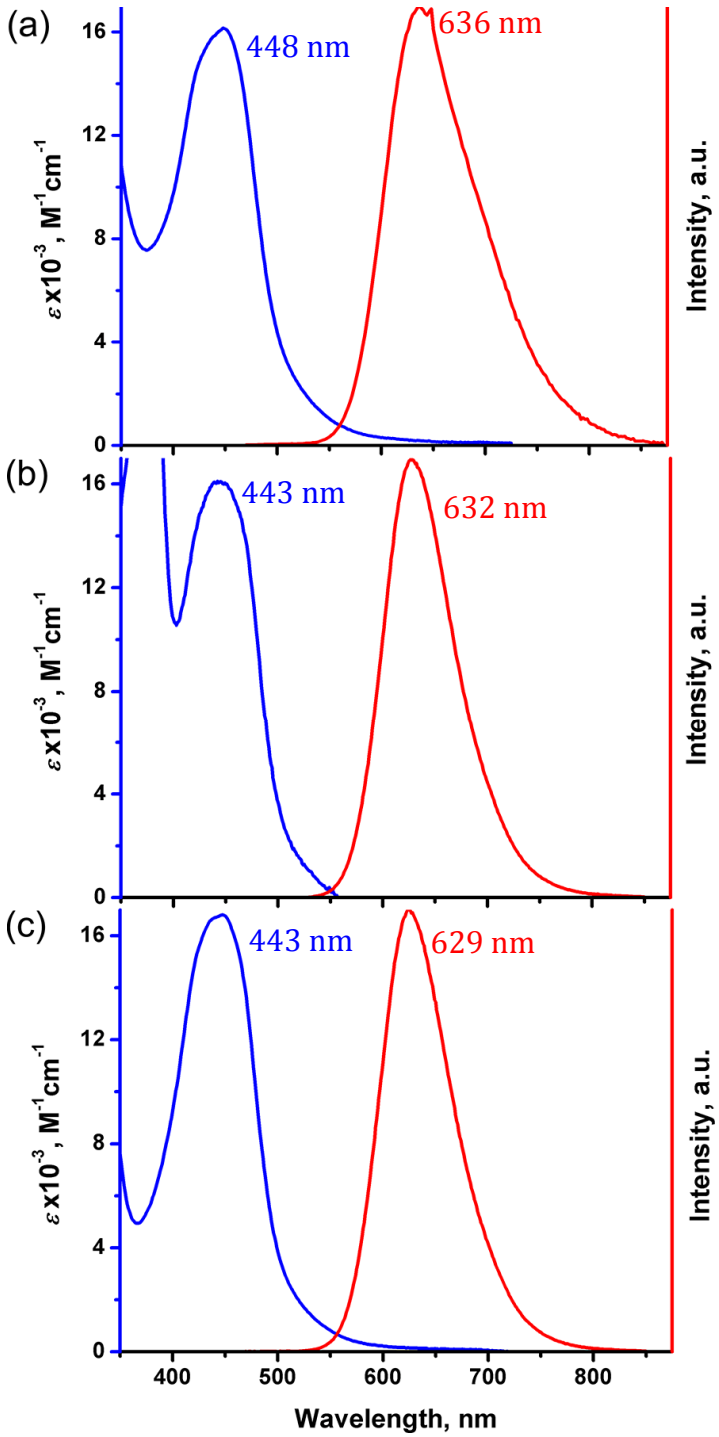

Figure S4. MLCT absorption bands and corresponding emission spectra of complexes **1-3** (a-c, respectively). The wavelengths of the absorption (λ_{abs}) and emission (λ_{em}) maxima are indicated.

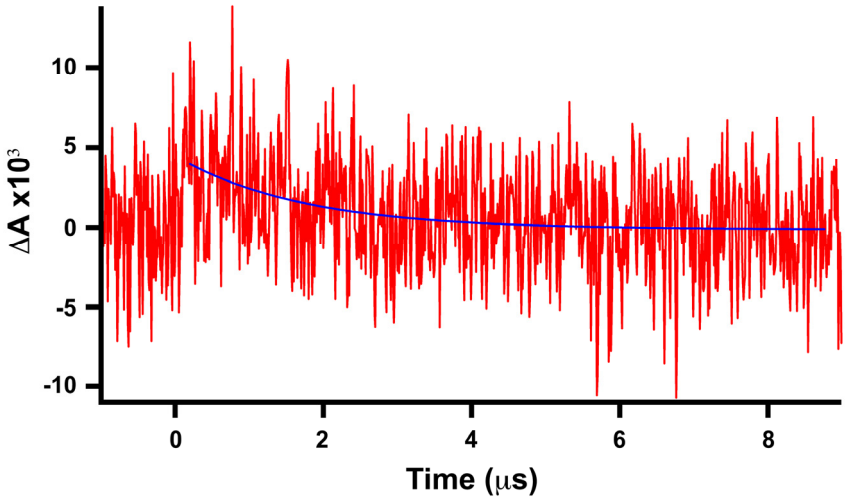

Figure S5. Kinetic profile of the difference absorbance spectrum of **1** in CH_3CN at room temperature. λ_{pump}=488 nm; λ_{probe}=370 nm. Red – experimental data; blue – single-exponential global fit.

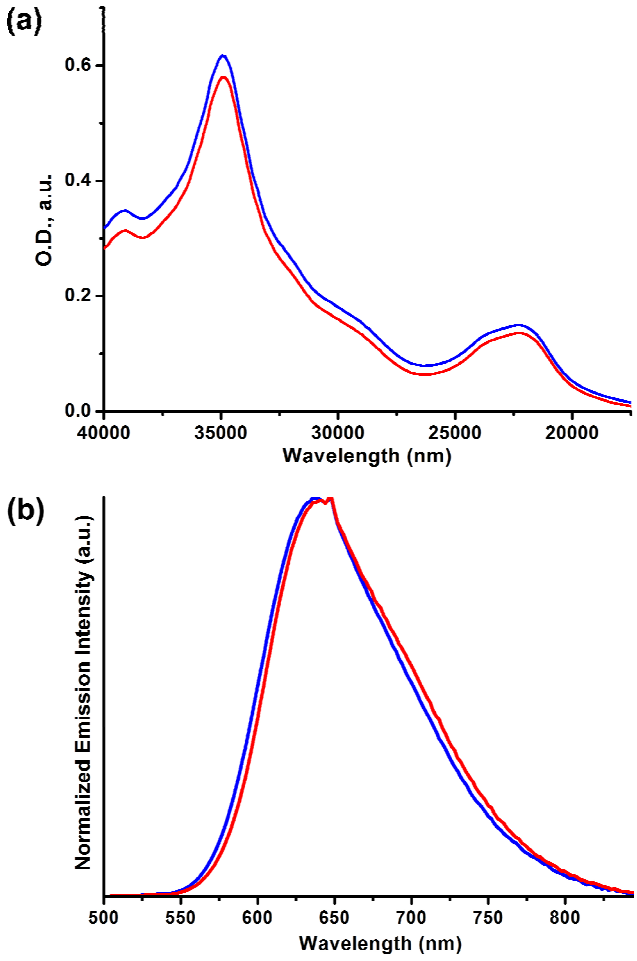

Figure S6. Absorption (a) and emission (b) spectra of **1** recorded on a solution prepared with freshly degassed CH_3CN (red) and on the same solution after keeping it in the dark for 4 hours (blue). Note that there is almost no difference between the absorption and emission bands of the two samples.